

First Principle Noncollinear Transport Calculation and Interfacial Spin-flipping of Cu/Co Multilayers

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In this paper the first principle noncollinear transport calculation for Cu/Co(111) including interfacial spin-flipping was performed. We modeled spin-flipping at the interface by assuming a noncollinear magnetic structure with random magnetization orientation which satisfied Gaussian distribution along average magnetization direction. The relationship between spin-dependent conductance including interfacial spin-flipping and random magnetization orientation distribution width was obtained. For certain distribution width, our defined spin-flipping ratio coincides with the range of experimental spin-flipping probability $P = 1 - e^{-\delta}$, where $\delta = 0.25 \pm 0.1$. The magnetoresistance in Co/Cu/Co spin valve system including interfacial spin-flipping has also been calculated.

I. INTRODUCTION

The electron transport across ferromagnetic/nonmagnetic (FM/NM) interface is of interesting in the past two decades.^{1,2,3} Based on the two current model(non spin-flipping theory), *ab initio* calculation with no-free parameter of interfacial specific resistance⁴ agreed reasonably well with experimental data for some lattice-matched metal pairs, such as fcc Cu(111)/Co(111)⁵ and bcc Fe(110)/Cr(110).⁶

The spin-flipping at the FM/NM interface, which certainly exists in the experiment, is not well studied, partially due to the theoretical difficult, and partially due to lacking of reliable experimental data.⁷ However, spin-flipping at the FM/NM interface is getting increasing importance. Spin-flipping at the ferromagnetic/suppperconductor interface can induce spin triplet pairing in the ferromagnetic side.^{8,9,10} In addition, the spin-flipping at the FM/NM interface can also change the spin torques induced by current.^{11,12,13}

Moreover, Geux *et al.* have calculated the transmission probability in the presence of magnetic impurity scattering with spin-flipping by the effective mass approximation.¹⁴ They calculated the transmission probability matrix in spin space and obtained that the spin-flipping probability is proportional to the impurity density. They also found that to the first order the calculated conductances from transmission probability matrix decrease linearly with increasing the impurity density. However, the transport properties through the real interface with interfacial spin-flipping process have not been studied yet.

In this paper, we will calculate the scattering matrix of real FM/NM interface with spin-flipping process by the first principle noncollinear transport calculation.¹⁵ The spin-flipping at the interface is modeled by assuming a noncollinear magnetic structure with random magnetization orientation which satisfied Gaussian distribution along average magnetization direction. By the noncollinear transport calculation,¹⁵ we can obtain how the interfacial conductance changes with random interfacial magnetic structure and the effect of interfacial spin-

flipping on the magnetoresistance in FM/NM/FM spin valve system.

II. COMPUTATIONAL DETAILS

Our calculation of scattering matrix is based on the surface Green's function method¹⁶ with tight-binding linear muffin tin orbital basis.¹⁷ First, the self-consistent one-electron effective potential in our calculation is obtained from collinear electron structure calculation¹⁶ without spin-orbit coupling. The Hamiltonian \hat{H}_0 is constructed by this self-consistent potential and is diagonal in spin space. Second, the rigid potential approximation has been used in our noncollinear transport calculation. In this approximation, we rotate the Hamiltonian \hat{H}_0 which is in local quantum axis representation in spin space to the global quantum axis representation. So the Hamiltonian for transport calculation can be written as $\hat{H}' = \hat{U}(\theta, \varphi) \hat{H}_0 \hat{U}^\dagger(\theta, \varphi)$, where $\hat{U}(\theta, \varphi)$ is the unity rotation matrix in spin space. θ and φ are the polar angle and azimuth angle of the local quantum axis respectively (global quantum axis is taken as z axis and $\varphi = 0$ in our calculations). Therefore the spin-flipping is only induced by interfacial magnetic disorder and the spin-orbit coupling is neglected in our transport calculation.

Due to the lack of the details of interfacial magnetic disorder, we assume that spin-flipping is introduced by the Gaussian random distribution of magnetization orientation. In our calculation all the magnetization orientation of Co atoms are along one global quantum axis except the Co monolayer at the interface. Further the disordered magnetization orientation is modeled by 10×10 lateral supercell. The deviation angles within the 10×10 supercell satisfy the Gaussian random distribution, where the average orientation is along global quantum axis and the distribution width is $\Delta\theta$. So the most deviation angles in the supercell are in the range of $(-\Delta\theta, \Delta\theta)$. However, the magnitude of magnetization for each Co atom in the supercell is constant. In this paper we have calculated the transport properties for different magnetization orientation distribution width, which is from $\Delta\theta = 0$ to

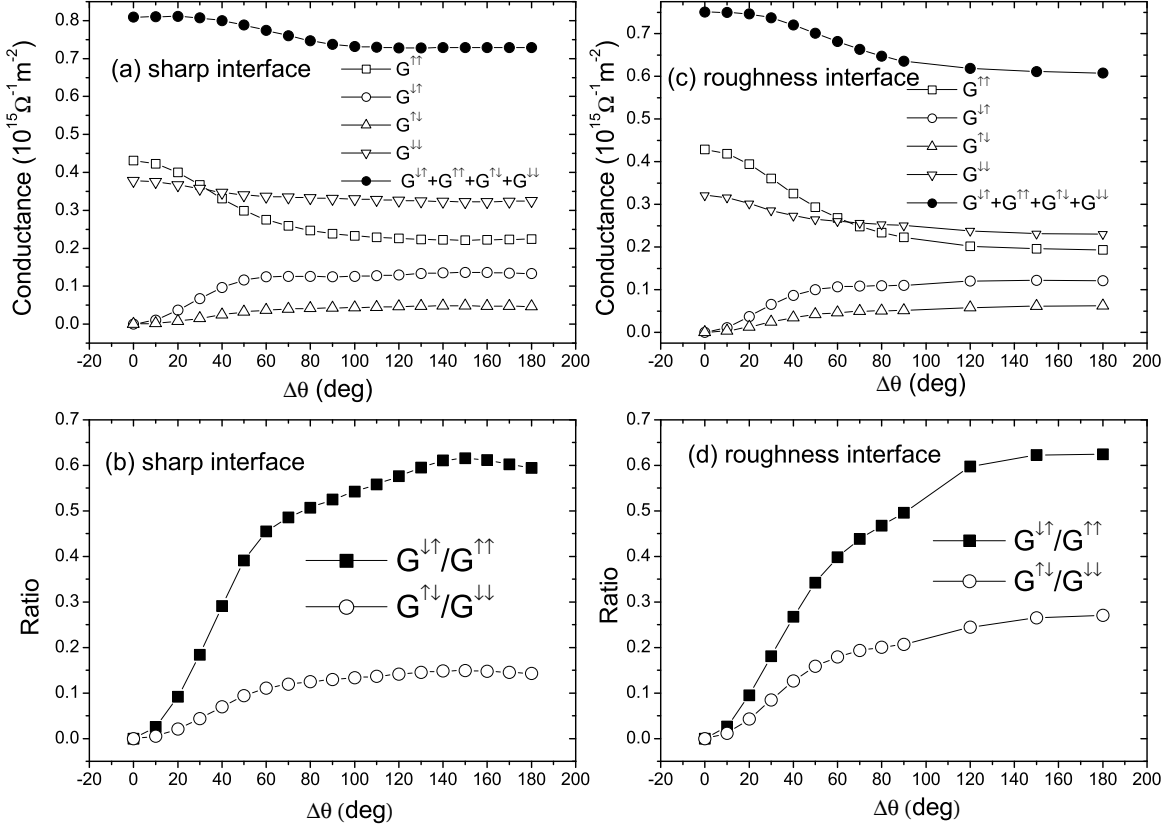


FIG. 1: The spin-dependent conductances of sharp and roughness Cu/Co(111) interfaces. (a) and (c) The conductances will be saturated for large $\Delta\theta$ case and the critical $\Delta\theta$ of roughness interface is larger than that of sharp interface. (b) and (d) For both sharp and roughness interface the spin in majority channel can be flipped more easily than that in minority channel.

180 (deg). Here the larger distribution width $\Delta\theta$ implies the larger probability of spin-flipping scattering process at interface.

The noncollinear magnetic structure at interface has been calculated by other group using first principle local spin density calculations,¹⁸ and the multiple and metastable noncollinear magnetic structure have been obtained in copper-permalloy interface. There are four metastable noncollinear states in which the energies are lower than the energy of collinear state or total random state. The collinearity of those four metastable states in their paper¹⁸ is in the range of about 0.4 to 0.8, which corresponds to our parameter $\Delta\theta \approx 40$ to 70 (deg).

III. RESULTS AND DISCUSSION

In our noncollinear Cu/Co(111) transport calculation the lattice constant is taken as $a=3.549\text{\AA}$. The spin-

dependent conductance is

$$G^{\sigma\sigma'} = \frac{e^2}{h} \sum_{\mu,\nu,\mathbf{k}_{\parallel}} T_{\mu\nu}^{\sigma\sigma'}(\mathbf{k}_{\parallel}) = \frac{e^2}{h} \sum_{\mu,\nu,\mathbf{k}_{\parallel}} |t_{\mu\nu}^{\sigma\sigma'}(\mathbf{k}_{\parallel})|^2 \quad (1)$$

where $t_{\mu\nu}^{\sigma\sigma'}$ is transmission matrix element for bloch state (ν, σ') in lead Cu to bloch state (μ, σ) in lead Co and \mathbf{k}_{\parallel} is lateral wave vector. Figure.1 shows the spin-dependent conductances with different magnetization orientation distribution width $\Delta\theta$, where the roughness interface is modeled by 2ML of 50%-50% alloy in a 10×10 lateral supercell, which can be denoted as $\text{Cu}[\text{Cu}_{0.5}\text{Co}_{0.5}|\text{Cu}_{0.5}\text{Co}_{0.5}]\text{Co}$. For this roughness interface the random Gaussian distribution of magnetization direction only takes place at the interfacial magnetic atoms (Co atoms). Here $G^{\uparrow\uparrow}$ and $G^{\downarrow\downarrow}$ are conductances for majority and minority electron channel with unchanging the orientation of spin. $G^{\uparrow\downarrow}$ ($G^{\downarrow\uparrow}$) is conductance for spin-flipping process, which describes the probability of majority (minority) being scattered to minority (majority).

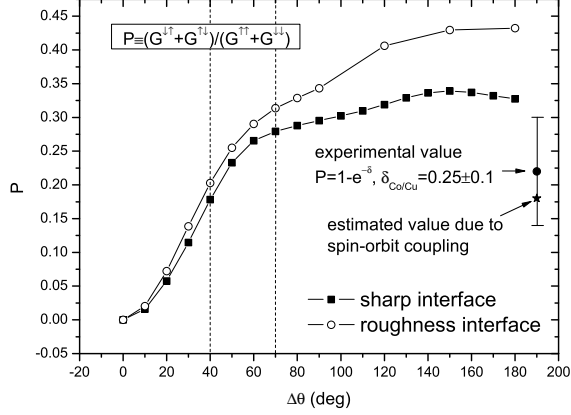


FIG. 2: The spin-flipping ratio across Cu/Co(111). The solid circle is the spin-flipping probability value $P = 1 - e^{-\delta} \approx 1 - e^{-0.25} \approx 0.22$ inferred from experiment data and the error bar comes from the uncertainty $\delta = 0.25 \pm 0.1$. The solid star is the estimated spin-flipping probability only due to the spin-orbit coupling. The range of $\Delta\theta$ between dash line corresponds to the collinearity 0.4 to 0.8 which is result of the magnetic structure calculation.

As shown in Figure.1(a) and (c), for both sharp and roughness interfaces, with increasing the magnetization direction distribution width $\Delta\theta$ the spin-flipping conductance increases and the majority (minority) conductance decreases more rapidly and the conductance $G^{\downarrow\uparrow}$ increases also more rapidly than $G^{\uparrow\downarrow}$. For sharp interface with increasing $\Delta\theta$, the total conductance ($G^{\downarrow\uparrow} + G^{\uparrow\downarrow} + G^{\uparrow\uparrow} + G^{\downarrow\downarrow}$) increases slightly at first and decreases to constant when $\Delta\theta > 90$ (deg). But for the roughness interface, the total conductance decreases monotonically and the critical distribution width $\Delta\theta$ where the conductance start to be saturated is about 120 (deg), which is larger than that for sharp interface. In our results of electron structure calculation, the average interfacial magnetic moment per atomic sphere is about $0.77\mu_B$ for roughness interface and $1.58\mu_B$ for sharp interface. Moreover for the same distribution of random interfacial magnetic structure, the larger interfacial magnetic moment will lead to more strongly spin-flipping scattering of the incoming electron. Therefore, it needs much more degree of interfacial magnetic structure disorder to saturate the conductance in the roughness interface.

In the case of non spin-flipping Cu/Co(111) interface the minority electron is reflected more strongly than the electron in majority channel. Taking into account the scattering induced by noncollinear magnetization, the conductances $G^{\uparrow\uparrow}$ and $G^{\downarrow\downarrow}$ both decrease with increasing $\Delta\theta$. Further the influence of noncollinear magnetization scattering is relatively more important for majority channel than for minority channel. Therefore as shown

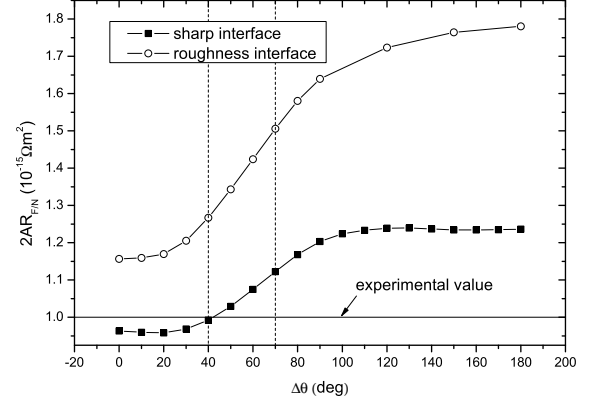


FIG. 3: The rounded interfacial specific resistance $2AR_{F/N}$ for different distribution width $\Delta\theta$, where the line in the figure corresponds to the value from the experiment. The region between two dash line corresponds to the result of magnetic structure calculation.

in Figure.1(a) and (c), $G^{\uparrow\uparrow}$ decreases more rapidly than $G^{\downarrow\downarrow}$. In addition, for both sharp and roughness interfaces we observe that $G^{\downarrow\uparrow}/G^{\uparrow\uparrow} > G^{\uparrow\downarrow}/G^{\downarrow\downarrow}$ in Figure.1(b) and (d), which also indicates that the spin in majority channel can be flipped more easily than that in minority channel.

The interfacial spin-flipping parameter δ usually describes the interfacial spin-memory-loss which is defined as $\delta = t_I/l_{sf}^I$ within VF theory,¹⁹ and the spin-flipping probability is⁷ $P = 1 - e^{-\delta}$. For Cu/Co interface $\delta \approx 0.25$ which is indirectly inferred by explaining the difference between 'interleaved' and 'separated' sample within VF theory.^{20,21,22} There is no direct measurement of parameter δ for F/N interface up to date and the value of δ inferred from experiment is quite uncertain.⁷ In this paper, we defined the spin-flipping ratio as $P \equiv (G^{\downarrow\uparrow} + G^{\uparrow\downarrow}) / (G^{\uparrow\uparrow} + G^{\downarrow\downarrow})$. From Figure.2 one can see that for $\Delta\theta \approx 40$ to 70 (deg) our defined spin-flipping ratio coincides with the range of spin-flipping probability inferred from experimental data ($P = 1 - e^{-\delta}$, $\delta = 0.25 \pm 0.1$).²⁰ This might be just an accident coincidence because we have not calculated the spin-flipping probability directly and our definition of the spin flipping ratio is only used for giving some quantitative information of spin-flipping. In addition, K. Eid *et al.*²⁰ estimated the interfacial spin-flipping probability at Cu/Co interface only due to the spin-orbit coupling and the result is $P = 1 - e^{-\delta} \approx 1 - e^{-0.2} \approx 0.18$, which is on the small side of the experimental P value range. The estimated spin-flipping probability due to spin-orbit coupling approximates the P value for the case of $\Delta\theta = 40$ (deg) in our calculation and is much smaller than the saturated spin-flipping probability due to magnetic disorder. Considering our calculation only taking the interfacial magnetic disorder into account, it is suggested that the

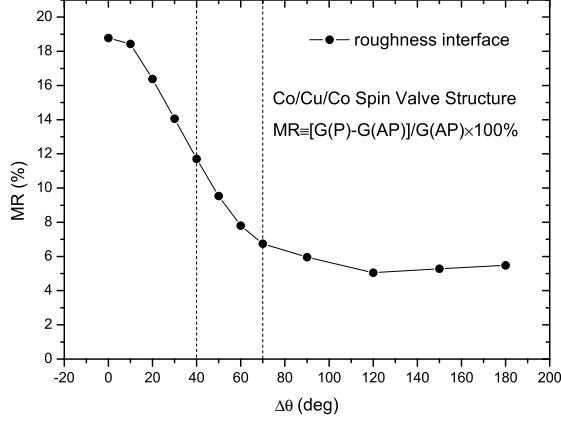


FIG. 4: The calculated MR of the spin valve system Co/Cu/Co with different interfacial spin-flipping, where the two Cu/Cu interfaces are both roughness with 2ML 50%-50% alloy. The region between two dash line also corresponds to the result of magnetic structure calculation.

spin mixing effect of interfacial magnetic disorder is more prominent than that of spin-orbit coupling on the Cu/Co transport properties, e.g. current-perpendicular-to-plane (CPP) magnetoresistance (MR).

Figure.3 shows the rounded interfacial specific resistance which is defined as²³

$$2AR_{F/N} = 2A \frac{h}{e^2} \left[\frac{1}{\sum T_{\mu\nu}^{\sigma\sigma'}} - \frac{1}{2} \left(\frac{1}{2N_{Cu}} + \frac{1}{N_{Co}^{\uparrow} + N_{Co}^{\downarrow}} \right) \right] \quad (2)$$

where A is section area, N_{Cu} , N_{Co}^{\uparrow} and N_{Co}^{\downarrow} are the Sharvin conductances. First, in non spin-flipping case for sharp interface we obtain $2AR_{F/N} \approx 0.96$ ($10^{-15}\Omega m^2$) which is close to the experimental value⁵ ~ 1.0 ($10^{-15}\Omega m^2$). Second, due to the additional scattering from noncollinear magnetization, with increasing $\Delta\theta$ the rounded interfacial specific resistance increases and for large distribution width the calculated $2AR_{F/N} \approx 1.23$ ($10^{-15}\Omega m^2$) which is about 128% of non spin-flipping specific resistance. Moreover the experimental specific resistance value corresponds to the case of $\Delta\theta \approx 40$ (deg) in our calculation, which indicates that the spin-flipping at interface can also explain the deviation of rounded interfacial specific resistance between sharp interface cal-

culation and experimental data. The rounded interfacial specific resistance of roughness interface is also shown in Figure.3. It can be seen that the specific resistance of roughness interface also increases with increasing $\Delta\theta$ as the case of sharp interface. However, the value of roughness interface is larger than that of sharp interface and the $\Delta\theta$ in which the specific resistance start to be saturated is also larger than that of sharp interface.

Figure.4 shows the magnetoresistance(MR) of the spin valve system Co/Cu/Co with roughness interface for different interfacial spin-flipping. We have calculated the conductances of the parallel $G(P)$ and antiparallel $G(AP)$ configuration, and the MR is defined as $MR \equiv \frac{G(P)-G(AP)}{G(AP)} \times 100\%$. One can observe that the MR decreases rapidly with increasing distribution width $\Delta\theta$ and for $\Delta\theta > 90$ (deg) the MR is nearly constant about 5%. For the region of $\Delta\theta = 40$ to 70 (deg) corresponding to the result of magnetic structure calculation,¹⁸ the MR is in range of 11.7% to 6.7%, which is about 2/3 to 1/3 of the non spin-flipping MR $\sim 18.8\%$.

IV. CONCLUSION

In this paper the first principle noncollinear transport calculation for Cu/Co(111) including interfacial spin-flipping was performed. We modeled spin-flipping at the interface by assuming a noncollinear magnetic structure with random magnetization orientation which satisfied Gaussian distribution along average magnetization direction. The relationship between spin-dependent conductance including spin-flipping conductance and random magnetization orientation distribution width was obtained. We found that the conductances start to be saturated when the distribution width $\Delta\theta$ larger than the critical width. For distribution width $\Delta\theta=40$ to 70 (deg) our defined spin-flipping ratio coincides with the range of spin-flipping probability $P = 1 - e^{-\delta}$, where $\delta = 0.25 \pm 0.1$ inferred from experimental data. In addition we also found that the magnetoresistance of Co/Cu/Co spin valve system decreases rapidly with increasing interfacial spin-flipping probability.

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